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# Electron Paramagnetic Resonance of d Transition Metal Compounds

by F.E. Mabbs and D. Collison, University of Manchester, Manchester, UK

Studies in Inorganic Chemistry Volume 16

Electron paramagnetic resonance (epr) spectroscopy is a sensitive and versatile method of studying paramagnets, which is finding increasing use in chemistry, biochemistry, earth and materials sciences.

The technique is treated both qualitatively and quantitatively, with a progressive increase in sophistication in each succeeding chapter. Following a general introductory chapter, the first half of the book deals with single unpaired electron systems and considers both metal and ligand Zeeman, hyperfine and quadrupole interactions. The simulation of these spectra is discussed, followed by the relationship between spin-Hamiltonian parameters and models of the electronic structures of paramagnets. The second half of the book treats multiple unpaired electron systems using the same philosophy. An introduction to the epr properties of cluster compounds and of extended exchanging systems is also given. There is a chapter on linewidths and lineshapes, and an extensive appendix containing much additional information. A wide-ranging library of simulated and experimental spectra is given, as well as graphical data which should aid spectrum interpretation. Each chapter contains key references and there is a substantial subject and keyword index.

This book is designed to teach epr spectroscopy to students without any previous knowledge of the technique. However, it will also be extremely useful to researchers dealing with paramagnetic d transition metals.

**Contents:** Preface. 1. The Electron Paramagnetic Resonance Experiment. 2. Spin Doublets in an Applied Magnetic Field: A Qualitative Treatment. 3. The Quantitative Description of the Spectra from Spin Doublets Interacting with an Applied Magnetic Field Only. 4. The Spectra from Spin Doublets Interacting with a Nuclear Spin: A Qualitative Treatment. 5. Spectra of Spin Doublets Interacting with a Nuclear Spin: A Quantitative Treatment. 6. Nuclear Quadrupole and Nuclear Zeeman Effects in Spin Doublets. 7. Spectrum Simulation for Spin Doublets. 8. Metal Ions in Cubic and Axial Ligand Fields. 9. The Relationship between the Spin-Hamiltonian Parameters and the Electronic Structures of Spin Doublet Paramagnets. 10. Paramagnets with  $S > 1/2$ . 11. Monomeric Spin Triplets: Qualitative and Quantitative Aspects. 12. Monomeric Spin Quartet Paramagnets. 13. Monomeric Spin Quintets: Qualitative and Quantitative Aspects. 14. Monomeric Spin Sextet Paramagnets. 15. Polynuclear Transition Metal Compounds. 16. Simulation of Spectra for Paramagnets with Multiple Unpaired Electrons. 17. Extended Electron Exchange in Crystals. 18. Relaxation, Linewidths, Determination of Concentrations, and Microwave Power Saturation. Appendices. Some

physical properties of selected solvents. Physical constants and conversion factors. Spin-Hamiltonians, operator equivalents and some relationships between angular momentum operators. Direction cosines and transformation of axes. Some useful mathematical relationships. Some properties of nuclei with non-zero nuclear spin and hyperfine interactions parameters. Polar coordinates, Cartesian coordinates, wavefunctions, orbitals. Determinantal wavefunctions. Inter-electron repulsion calculations. The effect of operators such as  $R^3/\delta x$ . Dipole-dipole interactions and the point-dipole approximations. Expanded FIR diagrams for  $S=1, 1, 3/2, 2, 5/2, 3, 7/2, 4, 9/2$ . Mean values of functions and the methods of moments. Subject and Keyword Index. Chemical Index.

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Progress In Research and Development of Processes and Products from Sols and Gels

Proceedings of the 2nd European Conference on Sol-Gel Technology,  
Saarbrücken, Germany, 2-5 June 1991

edited by S. Vilminot, R. Nass and H. Schmidt

European Materials Research Society Monographs Volume 5

Eurogel '91 is the second conference to report on the developments in research and technology of European laboratories and industry. The volume focuses on the scientific and technological progress in the field, as well as providing a global overview of the latest developments. The fifty presented papers report on many new themes and research groups.

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## Volume 6: Coadsorption, Promoters and Poisons

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The present volume provides particularly clear evidence of this growth. In the specific area of application of heterogeneous catalysis, substantial progress is being made in confronting problems of increasing complexity, such as those associated with *Coadsorption, Promoters and Poisons*, which forms the subject matter of this book. This progress is reflected in sophisticated theoretical calculations as well as experiments, and both areas are covered in chapters which are written by acknowledged experts in the field. Specific problems covered include the effect of

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The book should be of interest to the many researchers in the field of surface science (coming from backgrounds in chemistry, physics and materials science), as well as to those interested in heterogeneous catalysis.

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Adsorbates and Adsorbed Molecules (CO; H<sub>2</sub>O) (*H.P. Bonzel, G. Pirug*). Chapter 4. Coadsorption of Carbon Monoxide and Hydrogen on Metal Surfaces (*X.-C. Guo, D.A. King*). Chapter 5. Adsorption on Bimetallic Surfaces (*W.K. Kuhn, R.A. Campbell, D.W. Goodman*). Chapter 6. The Chemical Properties of Alloy Single Crystal Surfaces (*B.E. Nieuwenhuys*). Chapter 7. Promotion in Ammonia Synthesis (*M. Bowker*). Chapter 8. Promotion in the Fischer-Tropsch Hydrocarbon Synthesis (*R.W. Joyner*). Chapter 9. Promoters and Poisons in the Water-Gas Shift Reaction (*C.T. Campbell*). Chapter 10. Strong Metal-Support Interactions (*J.P.S. Badyal*). Index.

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